CCP4@DL: More than just a Software Suite!

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The Collaborative Computational Project No. 4 (CCP4) is based at Daresbury Laboratory and is one of the most successful of the Research Council supported CCPs. CCP4 is best known for distributing a suite of programs and software libraries which are used for macromolecular structure determination by X-ray crystallography. However, as this poster shows, the project engages in a range of other activities which aim to encourage communication and collaboration within the protein crystallography community.

CCP4 at Daresbury Laboratory

The core CCP4 staff at Daresbury Laboratory currently comprises 4 full-time scientific programmers plus a part-time administrative assistant, who helps to administer the day-to-day running of the project.

These staff are responsible for co-ordinating software development, providing user support and making the public releases of the software, in addition to organising the activities you see here. The CCP4 programmers also provide on-site user support for CLRC staff and SRS users.

CCP4 Study Weekend and Masterclasses

The annual Study Weekend is CCP4's flagship workshop, and is one of the largest conferences organised from Daresbury Laboratory. As such it is only made possible in a large part with the assistance of SRD administrative staff.

Each year around 450 delegates attend the 2-day workshop to hear internationally renowned speakers talk on the particular aspect of macromolecular crystallography chosen for that year. Students and young scientists are particularly encouraged to attend, and for many of them CCP4 provides financial support to make this possible.

Articles written by the speakers are collected into the Study Weekend Proceedings. Past proceedings were produced at Daresbury but since 1998 they have been published as special issues of *Acta Crystallographica D*.

Above: a session at the 1999 CCP4 Study Weekend

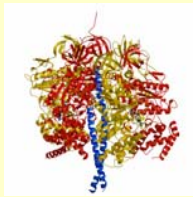
Closer to home, CCP4 is also organising a series of **Protein Crystallography Masterclasses** at Daresbury, in conjunction with the PX group at the Laboratory.

So far these have covered topics such as data processing, scaling, and refinement, and have focused on practical details, attracting attendees from both commercial companies and local universities.

The most recent of these talks has also been made available on-line from Daresbury (above, see http://www.ccp4.ac.uk/talks), registering over 500 viewers in the first 24 hours.

The CCP4 Software Suite

The structures of the light harvesting complex LH2 (left) and the "energy enzyme" F1-ATPase (below) were both determined from data collected at the Daresbury SRS, in a large part using the programs in the CCP4 Suite.



References:

LH2: *G. McDermott, S.M. Prince, A.A. Freer, A.M. Hawthornwaite-Lawless, M.Z. Papiz, R.J. Cogdell and N.W. Isaacs (1995)* Nature ***374****, 517-21*

F1-ATPase: *J.P. Abrahams, A.G.W. Leslie, R. Lutter and J.E. Walker (1994)* Nature ***370,*** *621-28*

The CCP4 software suite is at the core of the CCP4 project.

The suite comprises over a hundred programs covering all aspects of macromolecular structure solution, from processing of the initial diffraction images, through data reduction and phasing by MIR, MR, MAD and direct methods, to model refinement and analysis of the final structure. It has been used in countless structure solutions, just two of which are shown on the left.

Many of the programs are contributed and updated by the original authors, and new programs are constantly being added. CCP4 has also funded programmers to work on new and existing applications, for example the Maximum-Likelihood Refinement program REFMAC, and the Data Processing package MOSFLM.

The software is maintained by the Daresbury staff and is distributed from an FTP server at the Laboratory to nearly a thousand academic and industrial sites around the world.

Commercial Activities

Although the CCP4 software suite is provided free-of-charge to academics and not-for-profit organisations, commercial companies are required to pay a licence fee. Currently there are over 80 companies around the world using the software, ranging from small biotech start-ups to established pharmaceutical companies, resulting in commercial receipts of nearly half a million pounds per annum.

This money is used to fund development of new and existing software, which is included in future releases of the suite. It also enables CCP4 to finance many of the activities mentioned on this poster, most notably the annual Study Weekend.

CCP4 and the Crystallographic Community

Bulletin Boards and Newsletters

The CCP4 e-mail bulletin board **ccp4bb** is hosted at Daresbury and provides a lively forum for discussion on a wide range of topics in macromolecular crystallography. With over 1800 international subscribers, the bulletin board has become a valuable resource for crystallographers, with postings ranging beyond the use of CCP4 software, to encompass crystallisation and data collection techniques, refinement strategies and employment opportunities. See http://www.ccp4.ac.uk/ccp4bb.html for more information.

CCP4 also produces a twice-yearly Newsletter containing a mixture of news, program announcements, meeting reports and scientific articles of general interest to crystallographers. Paper copies of the newsletter are sent to around 350 groups around the world, and the most recent electronic version (available from http://www.ccp4.ac.uk/newsletters.html) has already registered over 1500 readers.

Workshops and Conferences

Each year CCP4 is represented in various ways at international workshops and conferences. Often CCP4 simply provides financial assistance to enable small meetings to go ahead (for example, the annual BCA PX Summer School), or more tangibly by CCP4 staff appearing in exhibitions at major international conferences (including the IUCr Congress in 1999, and the ACA and ECM annual meetings in 2000 and 2001) and as invited speakers at both scientific meetings and at educational workshops.

A recent example is the Protein Crystallography Data Collection Workshop, which was held at Daresbury in early 2001. The workshop received a financial contribution from CCP4, and two of the CCP4 staff gave talks and assisted with the practical sessions.

Above: CCP4 representatives, including two of the Daresbury staff, on the exhibition stand at the ACA meeting in 2000.

CCP4 Collaborations

CCP4 is involved in a number of collaborations both within and external to CLRC, including 3 European Union contracts.

AUTOSTRUCT is a European initiative bringing together software developers to develop new algorithms and improve the interoperability of different software packages.
DNA is a collaboration between European synchrotrons (including the SRS) to automate data collection and processing procedures.
CCP4 has strong links with the European Bioinformatics Institute (EBI), including an ongoing collaboration to improve structure validation and deposition procedures. This includes one joint appointment plus funding for a postdoctoral position at Daresbury.
CCP4 is also involved in two BBSRC e-science initiatives based at Daresbury, and has links with the NorthWest Structural Genomics Consortium (NWSGC).

The CCP4 project is supported by the BBSRC, by income from commercial distribution of the software and by CCLRC Daresbury Laboratory. CCP4 would also like to thank the many people who have contributed to the project since its inception. For more information about CCP4, please visit our web pages at http://www.ccp4.ac.uk/